AFRL-OSR-VA-TR-2015-0114

Tailoring high order time discretizations for use with spatal discretizations of hyperbolic PDEs

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05/19/2015
Final Report

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Air Force Research Laboratory
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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

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1. REPORT DATE *(DD-MM-YYYY)*
May 6, 2015

2. REPORT TYPE
Final Performance Report

3. DATES COVERED *(From - To)*
05/01/2012-4/30/2015

4. TITLE AND SUBTITLE

Tailoring high order time discretizations for use with spatal discretizations of hyperbolic PDEs

5a. CONTRACT NUMBER
FA9550-12-1-0224

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Sigal Gottlieb

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

AND ADDRESS(ES)

U. of Massachusetts
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

AFOSR

875 N RANDOLPH ST RM 3112

ARLINGTON, VA 22203

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT

	NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT DISTRIBUTION A.
13. SUPPLEMENTARY NOTES

14. ABSTRACT

The major accomplishment of the current research was to overcome the time-stepping constraints and the order barriers on explicit and implicit strong stability preserving methods. This was attained through the study of multi-step multistage methods, multi-derivative methods, methods of variable linear and nonlinear orders, and methods which include downwinding. The results of this work include four families of new SSP methods which break order barriers and time-step bounds of previously known methods.

15. SUBJECT TERMS

strong stability preserving methods, time discretizations, hyperbolic partial differential equations, Runge—Kutta methods, multistep methods,

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
					Sigal Gottlieb
a. REPORT	b. ABSTRACT	c. THIS PAGE	UU	5	19b. TELEPHONE NUMBER *(include area code)*
U	U	U			508-999-8205

Final Report
Grant/Contract Title: **Tailoring high order time discretizations for use with spatal discretizations of hyperbolic PDEs**
Grant Number: FA9550-12-1-0224
Sigal Gottlieb[1]

1 Abstract

Strong stability preserving (SSP) high order time discretizations were developed [6] to ensure nonlinear stability properties necessary in the numerical solution of hyperbolic partial differential equations with discontinuous solutions. SSP methods preserve the strong stability properties – in any norm, seminorm or convex functional – of the spatial discretization coupled with first order Euler time stepping, when the timestep is suitably restricted.

The major accomplishment of the current research was to overcome the time-stepping constraints and the order barriers on explicit and implicit SSP methods. This was attained through the study of multi-step multistage methods, multi-derivative methods, methods of variable linear and nonlinear orders, and methods which include downwinding. The results of this work include four families of new SSP methods which break order barriers and time-step bounds of previously known methods.

The first family of methods considered incorporates implicit and explicit multistep multistage methods. For implicit methods of this class, we found that while methods of order higher than six can be found, the time-step barrier cannot be overcome. This means that the maximal effective strong stability coefficient (i.e. the scaling of the forward Euler timestep divided by the number of stages) cannot exceed two. This restrictive bound makes this implicit family not efficient for use in applications. However, explicit methods of this class were found, through an optimization code we developed, of up to five steps and ten stages and of order up to ten. These methods were tested on several applications and their strong stability properties verified.

The second family of SSP methods considered were explicit Runge–Kutta methods with linear order up to twelve and nonlinear orders up to the optimal SSP order of four. The optimal methods of nonlinear order three have identical strong stability coefficients to the corresponding linear methods. These methods have strong stability coefficients that approach those of the linear methods as the number of stages and the linear order is increased. These methods are efficient for use with problems where the SSP properties and a high linear order are required, as the increased nonlinear order does not reduce the allowable time-step significantly if at all.

The third family of SSP methods studied involves the use of multiple stages and multiple derivatives. Sufficient conditions for strong stability preservation for multistage two-derivative methods were determined and an optimization problem formulated. This enabled the discovery of optimal explicit SSP multistage two-derivative methods of up to order five, thus breaking the SSP order barrier for explicit SSP Runge–Kutta methods. Numerical tests showed the sharpness of the SSP condition in many cases, and demonstrated the need for SSP time-stepping methods in simulations where the spatial discretization is specially designed to satisfy certain nonlinear stability properties.

The fourth family of SSP methods developed includes the use of a downwinding term. This term approximates the same spatial derivatives as the original operator, but satisfies the desired strong stability property when solved backward in time. The addition of downwind terms has allowed methods that exceed the time-step restriction typically seen for implicit Runge–Kutta methods. This work is continuing and is expected to yield both implicit and explicit methods that break the order barrier associated with SSP methods.

[1]Mathematics Department, University of Massachusetts Dartmouth

2 Major Accomplishments:

1. **Optimal implicit and explicit SSP k-step Runge–Kutta methods:** *Motivation:* Without the use of *downwinding*, explicit SSP Runge-Kutta methods are limited to fourth order and implicit SSP Runge-Kutta methods are limited to sixth order. SSP multi-step methods do not suffer from this order barrier, but have very restrictive SSP coefficients. Efficient explicit SSP methods of order greater than four are frequently desirable, particularly when dealing with high order spatial discretizations. General linear methods, which have multiple steps and multiple stages have the potential to combine the properties of multistep and Runge–Kutta methods, and so provide an advantage over these methods by allowing a larger step-size [3]. We have shown [2] that explicit general linear methods have a bound on the SSP coefficient which is equal to the number of stages. Even considering this bound, explicit general linear methods may be found that have order $p > 4$ and larger SSP coefficient than the multistep methods.

   Multistep Runge-Kutta methods are a straightforward generalization of Runge-Kutta and linear multistep methods, and take the form

$$\begin{aligned} y_i^n &= \textstyle\sum_{j=1}^k d_{ij} u^{n+1-j} + \Delta t \sum_{j=1}^s a_{ij} f(y_j^n), \quad 1 \le i \le s, \\ u^{n+1} &= \textstyle\sum_{j=1}^k \theta_j u^{n+1-j} + \Delta t \sum_{j=1}^s b_j f(y_j^n). \end{aligned}$$

   Here the values u^n denote solution values at the times $t = n\Delta t$, while the values y_j^n are intermediate stages used to compute the next solution value. We will also consider a simple generalization of these methods, based on the following reasoning. For some methods, it may happen that the row i of A is identically zero and row i of D is $(1, 0, \ldots, 0)$, so that $y_1^n = u^n$. Then the method involves $f(u^n)$, and at any step we will have computed already $f(u^{n+1-j})$ for $j = 1, \ldots, k$, so these values may as well be used in computing the next step. This leads to methods of the form

$$\begin{aligned} y_1^n &= u^n, \\ y_i^n &= \sum_{j=1}^k d_{ij} u^{n+1-j} + \Delta t \sum_{j=2}^k \hat{a}_{ij} f(u^{n+1-j}) + \Delta t \sum_{j=1}^s a_{ij} f(y_j^n), \qquad 2 \le i \le s, \\ u^{n+1} &= \sum_{j=1}^k \theta_j u^{n+1-j} + \Delta t \sum_{j=2}^k \hat{b}_j f(u^{n+1-j}) + \Delta t \sum_{j=1}^s b_j f(y_j^n). \end{aligned}$$

   This form is more suitable for finding explicit methods. In the past [4], we developed a MATLAB optimization code and found explicit SSP two-step Runge–Kutta methods of the form (2.1). In recent work, we found methods of up to five steps and ten stages and up to tenth order. We tested these methods on a variety of problems.

   The methods can be downloaded from our website `http://sspsite.org/msrk.html`. The paper has been submitted for publication and can be downloaded from `http://arxiv.org/abs/1307.8058`.

2. **Optimal explicit SSP Runge–Kutta methods with high linear order and optimal nonlinear order:** The search for high order strong stability time-stepping methods with large allowable strong stability coefficient has shown that explicit SSP Runge–Kutta methods exist only up to fourth order [1]. However, if we restrict ourselves to solving only linear autonomous problems, the order conditions simplify and this order barrier is lifted: explicit

SSP Runge–Kutta methods of any *linear order* exist. These methods reduce to second order when applied to nonlinear problems.

Under this grant, we developed an optimization code to search for explicit SSP Runge–Kutta methods with large allowable time-step, that feature high linear order and simultaneously have the optimal fourth order nonlinear order. A MATLAB code (based on [5]) was used for finding methods with maximal SSP coefficient among those with a given linear and nonlinear order and number of stages. Optimal methods of up to twelve stages and linear order twelve, and nonlinear order four were found. The optimal methods of nonlinear order three have identical strong stability coefficients to the corresponding linear methods, These methods have strong stability coefficients that approach those of the linear methods as the number of stages and the linear order is increased. This work shows that when a high linear order method is desired, it may be still be worthwhile to use methods with higher nonlinear order.

This work has been accepted for publication in *Mathematics of Computation* and is available for download on Arxiv at `http://arxiv.org/abs/1403.6519`.

3. **SSP analysis of multistep multiderivative time stepping methods**
   With the increasing popularity of multi-stage multiderivative methods for use as time-stepping methods for hyperbolic problems [7, 8], the question of their strong stability properties needs to be addressed. We developed sufficient conditions for strong stability preservation for multistage two-derivative methods: We assumed that, in addition to the forward Euler condition, the spatial discretization of interest satisfies a second derivative condition. With these assumptions in mind, we formulated an optimization problem which enabled us to find optimal explicit SSP multistage two-derivative methods of up to order five, thus breaking the SSP order barrier for explicit SSP Runge–Kutta methods. In numerical tests we showed the sharpness of the SSP condition in many cases, and demonstrated the need for SSP time-stepping methods in simulations where the spatial discretization is specially designed to satisfy certain nonlinear stability properties. Future work will involve building SSP multiderivative methods while assuming different base conditions and with higher derivatives. Additional work will involve developing new spatial discretizations suited for use with SSP multiderivative time stepping methods. These methods will be based on WENO or discontinuous Galerkin methods and will satisfy pseudo-TVD and similar properties for systems of equations.

   The paper describing this work, in collaboration with Andrew Chrislieb and David Seal, was submitted for publication and is available on Arxiv at `http://arxiv.org/abs/1504.07599`.

4. **Implicit Runge–Kutta time-stepping with downwinding** To more easily analyze SSP methods, we rewrite Runge–Kutta methods in the form:

$$
\begin{aligned}
u^{(0)} &= u^n, \\
u^{(i)} &= \sum_{k=0}^{i-1} \left(\alpha_{i,k} u^{(k)} + \Delta t \beta_{i,k} F(u^{(k)}) \right), \quad \alpha_{i,k} \geq 0, \qquad i = 1, ..., m \qquad (2.1) \text{ ?1.8?} \\
u^{n+1} &= u^{(m)}.
\end{aligned}
$$

   Explicit SSP Runge-Kutta methods are known to be limited to fourth order and implicit SSP Runge-Kutta methods are limited to sixth order. However, if we allow the use of negative coefficients $\beta_{i,k}$ it is possible to overcome this order barrier. The presence of negative coefficients requires the use of a modified spatial discretization for these instances. When $\beta_{i,k}$ is negative, $\beta_{i,k} F(u^{(k)})$ is replaced by $\beta_{i,k} \tilde{F}(u^{(k)})$, where $\tilde{F}$ approximates the same spatial derivative(s) as

F, but the strong stability property holds for the first order Euler scheme, solved backward in time. Numerically, the only difference is the change of the upwind direction.

A further problem is the bounds on the SSP coefficient of $\mathcal{C} \leq m$ for explicit methods and of $\mathcal{C} \leq 2m$ for implicit methods. Both the order barrier and the SSP coefficient bound may be alleviated by the use of SSP methods with downwinding. We have created an optimization code in MATLAB which seeks implicit methods with downwinding with a large allowable SSP coefficient and found methods of up to order $p = 5$ which have $\mathcal{C} >> 2m$. Explicit methods still have SSP coefficients limited by the bound, however we can find methods of higher order than four. This is an ongoing area of research and although we have made significant progress we expect to have more results over the course of the next grant.

5. **GPU optimized time-stepping modules:** We are currently creating GPU-optimized modules for the developed time-stepping methods, which include CPU implementation of the spatial discretization coupled with GPU implementation of the time-stepping method.

3 Other Information

Dissemination We continue to update our SSP RK web-site to disseminate the results of the study. This site serves as an online catalog of all the methods studied, noting which are most successful, and commenting on the theoretical properties of each, and on which performed best with which spatial approximation.

In February 2013, I organized two minisymposium sessions on SSP methods at the SIAM CSE meeting in Boston, and at the ICOSAHOM 2014 meeting in Utah I gave the opening plenary lecture on SSP methods and organized a multi-session minisymposium on *Aspects of Time-Stepping* which included presentations on some of this work. I presented the new work on multiderivative methods as part of Antony Jameson's 80th birthday symposium at Stanford University in November 2014. Zachary Grant presented both the Linear/Non-linear SSP Runge–Kutta methods and the multistage multiderivative work at the SIAM CSE 2015 meeting in Utah and at the RPI graduate student event in April 2014. He also presented the multistage multiderivative work at WPI and Tufts as part of the SIAM student chapter seminars.

Personnel Supported During Duration of Grant

Sigal Gottlieb, Professor of Mathematics, UMass Dartmouth.
Daniel Higgs, Graduate Student, UMass Dartmouth.
Zachary Grant, Undergraduate/graduate Student, UMass Dartmouth.
Sidafa Conde, Undergraduate/graduate Student, UMass Dartmouth.

Publications

1. A. J. Christieb, S. Gottlieb, Z. J. Grant, D. C. Seal "Explicit Strong Stability Preserving Multistage Two-Derivative Time-Stepping Schemes ." Submitted. Available on Arxiv at `http://arxiv.org/abs/1504.07599`

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Acknowledgment/Disclaimer This work was sponsored (in part) by the Air Force Office of Scientific Research, USAF, under grant/contract number FA9550-12-1-0224. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.

References

SSPbook [1] S. Gottlieb, D. I. Ketcheson, and C.-W. Shu, *Strong Stability Preserving Runge–Kutta and Multistep Time Discretizations*, World Scientific Press, 2011.

SSPreview2008 [2] S. Gottlieb, D.I. Ketcheson and C.-W. Shu. High Order Strong Stability Preserving Time Discretizations. *Journal of Scientific Computing* , **vol 38**, No. 3 (2009), pp. 251–289.

ketcheson2007 [3] D.I. Ketcheson, C.B. Macdonald and S. Gottlieb. Optimal implicit strong stability preserving Runge-Kutta methods. *Applied Numerical Mathematics*, doi: 10.1016/j.apnum.2008.03.034.

tsrk [4] D. I. Ketcheson, S. Gottlieb, and C. B. Macdonald, *Strong stability preserving two-step Runge-Kutta methods*, SIAM Journal on Numerical Analysis, (2012), pp. 2618–2639.

ketchcodes [5] D. I. Ketcheson, M. Parsani, and A. J. Ahmadia, *Rk-opt: Software for the design of Runge–Kutta meththods, version 0.2*. `https://github.com/ketch/RK-opt`.

shu1988b [6] C.-W. Shu. Total-variation diminishing time discretizations. *SIAM Journal on Scientific and Statistical Computing*, 9:1073–1084, 1988.

sealMSMD2014 [7] D. C. Seal, Y. Guclu, and A. J. Christlieb, *High-order multiderivative time integrators for hyperbolic conservation laws*, Journal of Scientific Computing, 60 (2014), pp. 101–140.

tsai2014 [8] A. Y. J. Tsai, R. P. K. Chan, and S. Wang, *Two-derivative Runge–Kutta methods for PDEs using a novel discretization approach*, Numerical Algorithms, 65 (2014), pp. 687–703.

1.

1. Report Type

Final Report

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Primary Contact Phone Number

Contact phone number if there is a problem with the report

401-751-9416

Organization / Institution name

University of Massachusetts Dartmouth

Grant/Contract Title

The full title of the funded effort.

Tailoring high order time discretizations spatial discretizations of PDEs

Grant/Contract Number

AFOSR assigned control number. It must begin with "FA9550" or "F49620" or "FA2386".

FA9550-12-1-0224

Principal Investigator Name

The full name of the principal investigator on the grant or contract.

Sigal Gottlieb

Program Manager

The AFOSR Program Manager currently assigned to the award

Fariba Fahroo

Reporting Period Start Date

05/01/2012

Reporting Period End Date

04/30/2015

Abstract

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http://arxiv.org/abs/1504.07599

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Changes in research objectives (if any):

Change in AFOSR Program Manager, if any:

Extensions granted or milestones slipped, if any:

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, $K)

	Starting FY	FY+1	FY+2
Salary			
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